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Vapor Pressure and Predicted Stability of American Contact Dermatitis Society Core Allergens

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Abstract

Background—Accurate patch testing is reliant on proper preparation of patch test allergens. The stability of patch test allergens is dependent on several factors including vapor pressure (VP).

Objective—This investigation reviews the VP of American Contact Dermatitis Society Core Allergens and compares stability predictions based on VP with those established through clinical testing.

Methods—Standard references were accessed for determining VP in millimeters of mercury and associated temperature in degrees celsius. If multiple values were listed, VP at temperatures that most approximate indoor storage conditions (20°C and 25°C) were chosen. For mixes, the individual component with the highest VP was chosen as the overall VP, assuming that the most volatile substance would evaporate first. Antigens were grouped into low (≤0.001 mm Hg), moderate (<1 to >0.001 mm Hg), and high (≥1 mm Hg) volatility using arbitrary cutoff values.

Conclusions—This review is consistent with previously reported data on formaldehyde, acrylates, and fragrance material instability. Given lack of testing data, VP can be useful in predicting patch test compound stability. Measures such as air-tight multidose reagent containers, sealed single-application dispensers, preparation of patches immediately before application, and storage at lower temperatures may remedy some of these issues.

Patch testing is critical in the diagnosis of allergic contact dermatitis. In the United States, T.R.U.E. TEST, which covers only a very limited of number of allergens, is the only patch test currently approved for use by the Food and Drug Administration. Comprehensive patch testing typically involves the use of commercially available allergens applied in Finn or IQ chambers. Commercially available allergens are typically prepared in either petrolatum or aqueous vehicles and packaged in syringes or bottles. There are 2 major conditions of concern regarding stability of allergens: (1) the stability of the reagent as supplied and stored according to manufacturer's instructions and (2) the stability of the reagent once placed in

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the patch test chambers. Unfortunately, these data are lacking for the majority of commercially available patch test allergens. Many patch testing allergens come not as pure substances but as mixtures consisting of solutes dissolved in a solvent or a colloid/suspension of 1 or more allergens dispersed in a vehicle such as water.

Several studies have evaluated stability of specific contact allergen reagents and were recently reviewed by Joy and colleagues.[1] These studies are summarized in Table 1 and include thiurams,[2] *p*-toluene diamine,[3] diisocyanates,[12,16] limonene hydroperoxide,[13] fragrances,[14,15] triglycidyl isocyanurate,[11] methyldibromo glutaronitrile,[5] acrylates,[9,10] corticosteroids,[8] as well as other allergens.[4,6,7,10] Data from these studies and others suggest that allergen vapor pressure (VP) is one of several important factors in predicting allergen stability. Volatility is the tendency for a nongaseous substance to vaporize spontaneously. This tendency can be measured in VP where the higher the VP, the more volatile the substance.[17] Greater volatility is thought to correlate with shorter shelf-life of a patch testing compound as more of it vaporizes from purchased stock or prepared solutions to the ambient air. Thus VP can be used as an approximation to stratify the stability of patch testing compounds in the absence of stability data. The purpose of this study was to document VPs of the American Contact Dermatitis Society (ACDS) Core Allergen Series.[18] The stability of patch test allergens in mixtures is a nonspecific term used to clinically mean how much of the allergen within the mixture is lost with time and not available for testing purposes. The source of this allergen loss is multifactorial and may include vaporization to air, chemical degradation, absorption into a porous storage container, and/or adsorption of an adherent film on container walls.

Methods

Chemical Abstract Series Registry (CAS) numbers were obtained from the *Chemotechnique Diagnostics*, Patch Test Products & Reference Manual 2014[19] and used to search for published VPs from the following online chemical databases: United States National Library of Medicine, National Center for Biotechnology Information, PubChem Open Chemistry Database,[20,21] Chemical Book [22] (an online data set of materials safety data sheets), and Chemical Laboratory Information Profiles[23] (a database of the American Chemical Society detailing physical and safety information on select chemical compounds originally published in the *Journal of Chemical Education*). Vapor pressure can be obtained from experimental data and estimated/extrapolated using the Antoine equation:[24]

$$log_{10} P = A - \frac{B}{C + T}$$

where P indicates vapor pressure; T indicates temperature; and A, B, and C indicate substance-specific constants.

Small discrepancies can be found between the databases, and when these were encountered, values from the PubChem followed by CLIP databases were utilized. Vapor pressure and associated temperature were recorded as millimeters of mercury and degrees celsius, respectively. If multiple VP values were listed, VP at temperatures that most approximate

indoor storage conditions (20°C and 25°C) were chosen. As VP varies nonlinearly with temperature per the Clasius-Clapeyron equation, VP at temperatures much higher than patch testing temperatures are largely irrelevant:[25]

$$\ln\left(\frac{P_1}{P_2}\right) = \frac{\Delta H_{\text{vap}}}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

where P indicates vapor pressure at T; T indicates temperature, ΔAH_{vap} indicates enthalpy of vaporization specific for substances; and R, gas constant (8.3145 J/(mol I K).

For allergen mixes, the individual component with the highest VP was chosen as the overall VP, based on the assumption that the most volatile substance would evaporate first. Documented VPs less than 0.001 mm Hg were listed as <0.001 mm Hg and assumed to be clinically equivalent.

Given the ambient and mild conditions during patch testing, it is unlikely that solid compounds will sublimate from solid to gas phases. Thus, VP was not useful with solids in suspension or compounds that do not dissolve in the vehicle.[26] Some metals salts are not soluble in petrolatum (eg, nickel sulfate), and therefore, VP is not helpful in predicting stability. To be comprehensive, we included VP for all allergens in the ACDS Core Allergen Series, including metal salts.

There are few established guidelines for volatility, and as such, categorical cutoff values for volatility are subjective [27]; relevance for patch test preparations is the amount of intact allergen present in the patch test chamber, and the temperature in which patch testing is usually performed. After discussion, we used the consensus cutoff values of 1 mm Hg or higher for high volatility, less than 1 to greater than 0.001 mm Hg for moderate volatility, and 0.001 mm Hg or less for low volatility at 25°C given data availability.

Results

Table 2 lists data for the ACDS Core Allergens with published VPs organized within categories of high, medium, and low volatility in alphabetical order. Data for acetone, ethanol, and water vehicles were included as reference points. Allergens with VP data at high temperatures were included if data were not available at ambient or near-ambient temperatures. Allergens without reported VPs were excluded from Tables 2 and summarized in Table 3. For mixtures, available data for each of the components were listed but for the purpose of stratification, the component with the highest VP was used as the overall VP. However, concentration of individual components of a mixture (eg, fragrance mix I) is not reported by the supplier.[19]

Volatile Allergens

Based on VP alone, the following allergens are predicted to be the least stable (high volatility): formaldehyde, acrylates (hydroxyethyl methacrylate, ethyl acrylate, and methyl methacrylate), sorbitan sesquioleate, glutaraldehyde, N,N-diphenylguanidine, and 3-

(dimethylamino)-1 propylamine (DMAPA). Those with moderate volatility include propylene glycol, methylisothiazolinone, fragrance-related allergens (benzyl alcohol, citral, cinnamic aldehyde, cinnamal, eugenol, citronellol, isoeugenol, cinnamyl alcohol, amyl cinnamal, and geraniol), phenoxyethanol, and chloroxylenol.

Nonvolatile Allergens

The following allergens are predicted to be relatively stable (>0.001 mm Hg VP): formaldehyde-related allergens (quaternium-15, DMDM hydantoin, tosylamide formaldehyde resin, bronopol), paraben mix constituents, rubber allergens (carba mix ingredients and N,N-diphenyl-*p*-phenylenediamine), 2 fragrances (coumarin and farnesol), 3 sunscreens (benzophenone-3 and -4 as well as 2-ethylhexyl-4-methoxycinnamate), and also benzocaine, epoxy resin, *p*-phenylenediamine (PDA), methyldibromoglutaronitrile, cetyl alcohol, stearyl alcohol, triclosan, and tocopherol.

Discussion

This study documents the VPs of ACDS Core Allergens. While the most conclusive studies involve analysis of “in use” allergens and patch test preparations, these data are not available for most allergens. The information published herein provides additional information to clinicians regarding 1 parameter that may affect the stability of common allergens. The volatility of an allergen should also be considered when compounding allergens within the dermatology clinic for diagnostic use.

Vapor pressure is defined by the Occupational Safety and Health Administration of the US Department of Labor in the Code of Federal Regulation as “a measure of a liquid's propensity to evaporate. The higher the VP, the more volatile the liquid and, thus, the more readily the liquid gives off vapors.” [17] More theoretically,it is the pressure of a vapor in thermodynamic equilibrium with its condensed phases (liquid and solid)in a closed system.In such a system, although there is constant change among the gaseous, liquid, and solid phases; there is no net change. Another way to think about VP is that it essentially measures the tendency for an atom or molecule to escape into the gaseous phase from condensed phases.[26] For example, a vacuum container, at time 0, contains liquid waterat20°C. Because the VP of liquid water at 20°C is approximately 760 mm Hg and the ambient pressure is 0 (vacuum), liquid water will immediately vaporize until VP is achieved or all of the liquid water has vaporized, whichever occurs first. Once at equilibrium, any additional application of energy such as heat will cause the liquid phase to change into gas phase, forming gas bubbles. As VP varies positively with volatility, the higher the VP, the higher the volatility and the higher the rate of loss of the substance from condensed to gaseous states.[17]

Based on our findings on VP alone, formaldehyde, acrylates (hydroxyethyl methacrylate, ethyl acrylate, and methyl methacrylate), and propylene glycol were predicted to have shorter shelf lives. This is consistent with previous research. Siegel et al[10] found that formaldehyde content measured in reagents obtained from a single patch test clinic and directly from the supplier was consistent with the label stated content upon receipt at the laboratory. Upon re-assay after 1 year of undisturbed storage under refrigerated conditions,

the formaldehyde reagents supplied in a syringe container had formaldehyde losses of 41% and 67%, while that supplied in an opaque plastic dropper had lost 31% of the formaldehyde from the water vehicle. While significant losses were observed for both container types, this preliminary observation suggests that a more air-tight container may help preserve volatile allergen integrity. The Antoine and Cassius-Clapeyron equations and other theories of thermodynamics were developed under the assumption of a closed system at equilibrium.[24–26] In real-world conditions, such as with patch testing compound storage and use, a closed system is not realistic; however, a pseudo-steady state can be achieved. With semiclosed systems such as a leaky container, steady state would be achieved where there is a steady diffusion of volatile gasses from the counter but with minimal change in the partial pressure within the container. This only occurs if there is an equal loss of patch test compounds from the solution to the gas. Thus, with time, there can be significant losses, especially if VP is high, providing a rationale for more air-tight storage methods.

Issues with acrylate allergen stability, specifically methyl methacrylate, were first documented by Kanerva et al.[28] They documented false-negative or questionable patch test results with methyl methacrylate obtained from 2 different manufacturers; one had nondetectable methyl methacrylate levels and the other only 25% of the labeled amount. Goon et al[9] studied methyl methacrylate stored in syringes and IQ chambers. They documented that methyl methacrylate stored in syringes at room temperature lost more than 20% of the labeled concentration within 2 weeks. When stored at −16°C, the loss was less than 20% at day 128, but increased to more than 20% of the initial concentration by 6 months. Loss was more rapid in IQ chambers under all conditions. Hypothesized reasons included evaporation or spontaneous polymerization. Siegel et al documented that the concentration of methyl methacrylate in stored syringes varied from the tip to the plunger of the syringe. The concentration at the tip of the syringes averaged 42% less than subsequent aliquots, suggesting that the major source of loss was due to volatility.[10] In addition, both Goon et al[9] and Siegel et al[10] observed significant loss of methyl methacrylate during compounding with petrolatum. During this process, petrolatum must be heated to higher than 65°C to melt the petrolatum, which can cause significant loss of allergen from volatilization as VP increases nonlinearly to increasing temperature.

Based on VP, volatility should not be a factor in the stability of paraben mix constituents, rubber allergens (carba mix ingredients and N,N-diphenyl-*p*-phenylenediamine), 2 fragrances (coumarin and farnesol), and 3 sunscreens (benzophenone-3 and -4 as well as 2-ethylhexyl-4-methoxycinnamate), and also benzocaine, epoxy resin, methyldibromoglutaronitrile, cetyl alcohol, stearyl alcohol, and tocopherol. This is consistent with previous publications. Gruvberger et al[5] tested 4 different concentrations of methyldibromoglutraonitrile at 1 year and found that all 4 were stable. Both patients tested to 40-year-old benzocaine, and 3 of 4 patients tested to 40-year-old epoxy resin reacted on patch testing.[6] We found no previous reports of stability testing to paraben mix, carba mix, coumarin, farnesol, cetyl alcohol, stearyl alcohol, sunscreens, or tocopherol.

Limitations

There are several limitations to these data. Vapor pressure data were unavailable for many ACDS core allergens. Also, numerous assumptions were made with regards to volatility and stability. First, VP is only one of the many chemical and physical aspects of allergen formulations, which may affect the accuracy of patch testing: self-polymerization, air reaction (including oxidation), carrier incapability, irritation, percutaneous penetration, as well as the presence of stabilizers or components within the mixes that may alter patch test results.[29,30] For example, based on VPalone, PDA has very low volatility at 25°C. However, it is very unstable in aqueous preparations as it is readily air oxidized to a brown heterogeneous mixture, whereas it is stable in petrolatum, likely due to protection from air.[31,32] Moreover, the vehicles themselves, as well as other constituents of a patch test preparation will likely contribute to the real-world volatility of a substance and potentially alter the patch test article stability.

Second, VP is based on the pure/neat chemical and thermodynamic equilibrium, not real-world conditions where solvent and other solutes may alter the volatility of the allergen. Third, there are few standard data on what cutoff value imparts “stability.” The World Health Organization made a determination between a very volatile organic compound, volatile organic compound, and semivolatile organic compound based on a substances' boiling point and not VP.[33] Boiling point is related to both vapor and atmospheric pressure, with the higher the VP, the lower the boiling point at a given atmospheric pressure. Finally, many ACDS Core Allergens are mixtures; overall VP could be affected by the partial pressures of each component, the interactions of each component with other components and/or with the solvent. We made the assumption that the stability of a mixture was that of the most volatile component.

Summary

This review provides additional information to clinicians on potential stability issues based on VP and is consistent with previously reported data on the instability of formaldehyde, acrylates, and fragrance materials. Specific reported stability data for a given allergen supersedes predictions based on VP. However, given the lack of experimental stability data of patch testing compounds, reliance on VP as a proxy for volatility may be a helpful tool for clinicians when compounding a patch test reagent or assessing the probability of a potential false-negative test.

The stability of commercial patch test allergens continues to be of concern as it impacts not only clinical diagnostic accuracy but also reliability of epidemiologic data reported in the literature. Potentially, patch test reagent stability/storage issues due to volatility may be minimized by use of more air-tight multidose reagent containers, sealed single application dispensers, storage at lower temperatures, and reliable beyond-use date labeling of multidose containers by patch test reagent suppliers. In addition, in an effort to minimize risk of false-negatives, allergens known to be highly volatile such as fragrances and those within the predicted high and medium volatility range should not be aliquoted and prepared until just before the application.

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Table 1

Publications Documenting Allergen Stability by Chemical Concentration Analysis or Clinical Testing

Reference, Allergen(s)	Conditions	Results
Bergendorff and Hansson[2]	Fresh, 3 mo	Concentration: NP Clinical: Tested 10 known thiuram-sensitive patients, all reacted to both
Thiuram		
Geier et al[3]	Fresh, 2 mo, 6 mo, 21 mo	Concentration: 1% fresh; 0.2% 2 mo; 0.1% 6 mo; 0.01% 21 mo Clinical: Tested 177 patients; 24 reacted to ≥1 κ = 0.81–0.86 (very good); 1 patient +++ 9 mo and negative to 14 mo and 18 mo; 4 patients + 2–11 mo
p-Toluene diamine		
Lembo et al[4]	Fresh, 6 y	Concentration: Thin layer chromatography testing acceptable Clinical: Tested 26 sensitized patients (1–7/allergen) All reacted to both
Balsam of Peru		
Cobalt		
Colophony		
Ethylenediamine		
Mercaptobenzothiazole		
Nickel		
Potassium dichromate		
Vioform		
Disperse yellow 3		
Formaldehyde		
Gruvberger et al[5]	Fresh, 1 y (4 concentrations)	Concentration: All 4 identical concentration; no degradation Clinical: NP
Methyldibromo glutaronitrile		
Bar et al[6]	40 y	Concentration: NP Clinical: 15 known positive patients tested Paraphenylenediamine, 5/5 patients positive Benzocaine, 2/2 patients positive Balsam of Peru, 1/3 patients positive Epoxy, 3/4 patients positive
Paraphenylenediamine		
Benzocaine		
Balsam of Peru		
Epoxy		
Mose et al[7]	2 h, 8 h, 24 h, 48 h, 72 h, 7 d	Concentration: Cinnamal (50% Fridge; 90% RT) Eugenol (30% Fridge; 75% RT) Van der Bend: 980% Fridge and RT ok MMA (960% Fridge; 0% RT) 2-HEMA (960% Fridge; 0% RT) 2-HPA (ok Fridge; 960% RT) Van der Bend: G20%; all 3 Fridge ok Clinical: NP
Cinnamal	RT, Fridge	
Eugenol	IQ, IQ Ult, Van der Bend	
MMA		
2-HEMA		
2-HPA		
Isaksson et al[8]	1y	Concentration: Tixocortol pet and eth, stable all conditions Budesonide pet and eth, stable all conditions Hydrocortisone-17 butyrate eth, freezer ok; RT e 3 mo Clinical: NP
Tixocortol	Pet, Eth	
Budesonide	RT, Fridge, Freezer	
Hydrocortisone-17 butyrate		
Goon et al[9]	4 mo	
2-HEMA	RT, Fridge, Freezer	Concentration: 2-HEMA, EGDMA, TREGDAVall temperatures ok

Reference, Allergen(s)	Conditions	Results
EGDMA TREGDA MMA 2-HPA	IQ, Finn	MMA 8 d RT, 10 d Fridge 2-HPA 21 d RT, 3 mo Fridge All rapid loss in IQ Clinical: NP
Siegel et al[10] MMA 2% Nickel Formaldehyde Glutaraldehyde 1%	In-use, unexpired and expired, allergens from patch test clinics	Concentration: Nickel, acceptable concentration Formaldehyde, acceptable concentration but loss occurred with storage Methyl methacrylate e56% Glutaraldehyde 27% to 45% Clinical: NP
Erikstam et al[11] Triglycidyl isocyanurate	3y	Concentration: 30% Clinical: Patient tested negative to allergen but positive to product
Frick-Engfeldt et al[12] MDI (diphenylmethane-4,4-diisocyanate) PMDI (polymeric diphenylmethane diisocyanate)	1y RT, Fridge, Freezer	Concentration: MDI failed all 3 PMDI better, but only freezer acceptable Clinical: NP
Nilsson et al[13] D-limonene	6 wk	Concentration: Oxidation products unstable α-Tocopherol stabilizer in pet causes degradation of hydroperoxides Use nonstabilized oxidized D-limonene Good for 6 wk Clinical: NP
Mowitz et al[14] Fragrance mix I Components	0, 4, 8, 24, 72, 144 h RT, Fridge 20 mg Finn open 30 mg IQ with plastic cover	Concentration: All Fridge 9 RT 4/7 decreased by 920% within 8 h at RT All except amyl cinnamal decreased by 920% by 144 h F Slightly better in FM than individually Clinical: NP
Hamann et al[15] Lyral	0, 8 h, 9 d 5 -C, 25 -C, 35 -C	Concentration: 8 h, ok 9 d 7 decreased by 30% at 35 -C; decreased by10% at 25 -C; decreased G5% at 5 -C Clinical: NP

RT, room temperature; Pet, petroleum; Eth, ethanol; NP, not performed.

Table 2

ACDS Core Allergens in Grouped by Volatility and in Alphabetical Order[19–23]

ACDS Core Allergen	CAS Number	VP, mm Hg	Temperature,°C	Database
High volatility (VP >1 mm Hg)				
3-(Dimethylamino)-1 propylamine	109-55-7	5	20	Chem book
Ethyl acrylate	140-88-5	38.6	25	Chem book
		9.98	30	PubChem
Formaldehyde	50-00-0	3890	25	PubChem
Glutaraldehyde	111-30-8	17	20	PubChem
Methyl methacrylate	80-62-6	29	20	PubChem
		38.5	25	
N,N-Diphenylguanidine	102-06-7	1.26	20	PubChem
Sorbitan sesquioleate	8007-43-0	42	20	Chem book
Vehicle, acetone	67-64-1	184	20	Chem book
		231	25	PubChem
Vehicle, ethanol	64-17-5	43.5	20	PubChem
Vehicle, water	7732-18-5	17.5	20	CLIP *
Medium volatility (VP <1 to >0.001 mm Hg)				
2,6-Ditert-butyl-4-cresol (BHT)	128-37-0	0.01	20	PubChem
4-Chloro-3-cresol (PCMC)	59-50-7	0.005	20	PubChem
Amyl cinnamal (fragrance mix I)	122-40-7	0.004	25	PubChem
Benzyl alcohol	100-51-6	0.099	20	PubChem
		0.094	25	
Chloroxylenol (PCMX)	88-04-0	0.002	25	PubChem
Cinnamal (cinnamic aldehyde in fragrance mix I)	104-55-2	0.029	25	PubChem
Cinnamyl alcohol (fragrance mix I)	104-54-1	<0.01	25	Chem book
Citral (fragrance mix II)	5392-40-5	0.091	25	PubChem
Citronellol (fragrance mix II)	106-22-9	0.02	25	PubChem
Ethyl cyanoacrylate	7085-85-0	0.31	20	PubChem
		<2	25	
Eugenol (fragrance mix I)	97-53-0	0.022	25	PubChem
Hydroxyethyl Methacrylate	868-77-9	0.126	25	PubChem *
Isoeugenol (fragrance mix I)	97-54-1	0.014	25	PubChem
Geraniol (fragrance mix I)	106-24-1	0.03	25	PubChem
Methylisothiazolinone	2682-20-4	0.062	25	PubChem
Phenoxyethanol	122-99-6	0.01	20	PubChem
		0.007	25	
Propylene glycol	57-55-6	0.08	20	PubChem
		0.13	25	
Sorbic acid	110-44-1	0.01	20	Chem book
Low volatility (VP <0.001 mm Hg)				
2-Bromo-2-nitropropane-1,3-diol	52-51-7	<0.001	20	PubChem

ACDS Core Allergen	CAS Number	VP, mm Hg	Temperature,°C	Database
1,3-Diphenylguanidine (carba mix)	74-31-7	<0.001	25	PubChem
2-Ethylhexyl-4-methoxycinnamate	5466-77-3	<0.001	25	PubChem
Benzocaine	94-09-7	<0.001	25	PubChem
Benzophenone-3 (2-hydroxy-4-methoxybenzophenone)	131-57-7	<0.001	25	PubChem
Benzophenone-4 (2-hydroxy-4-methoxybenzophenone-5-sulfonic acid)	4065-45-6	<0.001	25	PubChem
Butylparaben (paraben mix)	94-26-8	<0.001	25	PubChem
Cetyl alcohol (cetyl stearyl alcohol mix)	36653-82-4	<0.001	25	PubChem
Cobalt(II) chloride hexahydrate	7791-13-1	<0.001	25	CLIP *
Coumarin (fragrance mix II)	91-64-5	<0.001	25	PubChem
DL α-tocopherol	10191-41-0	<0.001	25	PubChem
DMDM hydantoin	6440-58-0	<0.001	25	PubChem
Epoxy resin-bisphosphenol A	1675-54-3	<0.001	25	PubChem
Ethylparaben (paraben mix)	120-47-8	<0.001	25	PubChem
Farnesol (fragrance mix II)	4602-84-0	<0.001	25	PubChem
Iodopropynyl butylcarbamate †	55406-53-6	<0.001	30	PubChem
Methyldibromoglutaronitrile	35691-65-7	<0.001	25	PubChem
Methylparaben (paraben mix)	99-76-3	<0.001	25	PubChem
p-Phenylenediamine †	106-50-3	<1	21	PubChem
		1.08	100	
Propylparaben (paraben mix)	94-13-3	<0.001	25	PubChem
p-tert-butylphenol (p-tert-butylphenol formaldehyde resin) †	98-54-4	0.23	50	PubChem
Quaternium-15	51229-78-8	<0.001	25	PubChem
Stearyl alcohol (cetyl stearyl alcohol mix)	112-92-5	<0.001	25	PubChem
Tetraethyl thiuram disulfide (carba mix)	97-77-8	<0.001	25	PubChem
Tetramethyl thiuram disulfide (carba mix)	137-26-8	<0.001	25	PubChem
Tosylamide (tosylamide formaldehyde resin)	70-55-3	<0.001	25	PubChem
Triclosan	3380-34-5	<0.001	20	PubChem

Vapor pressure listed with a maximum of 3 significant figures. VP < 0.001 mm Hg considered as negligible.

* Discrepancy between PubChem, CLIP, and/or Chem book.

† Data not available at 20°C or 25°C but available at much higher temperatures. Assumed low volatility since VP low at high temperatures.

Table 3

ACDS Core Allergens for Which VP Data Were Not Available[19–23]

ACDS Core Allergen Nickel(II) sulfate hexahydrate	CAS Number 10101-97-0	Comments
Myroxylon pereirae	Not available	
Hydroxycitronellal (fragrance mix 1)	107-75-5	Data from other components of fragrance mix 1 available
Oakmoss absolute (fragrance mix 1)	90028-68	Data from other components of fragrance mix 1 available
Neomycin sulfate	1405-10-3	
Budesonide	51333-22-3	
p-tert-butylphenol formaldehyde resin	Not available	Data for *p*-tert-butylphenol used
Potassium dichromate	7778-50-9	
Zinc dibutyldithiocarbamate (carba mix)	136-23-2	Data from other components of carba mix available
Zinc diethyldithiocarbamate (carba mix)	14324-55-1	Data from other components of carba mix available
Dipentamethylene thiuram disulfide (thiuram mix)	94-37-1	Data from other components of (thiuram mix available
Tetramethyl thiuram monosulfide (thiuram mix)	97-74-5	Data from other components of thiuram mix available
Diazolidinyl urea	78491-02-8	
N-cyclohexyl-N-phenyl-4-phenylenediamine (black rubber mix)	101-87-1	Data from other components of black rubber mix available
N-isopropyl-N-phenyl-4-phenylenediamine (black rubber mix)	101-72-4	Data from other components of black rubber mix available
Imidazolidinyl urea	39236-46-9	
N-cyclohexyl-2-benzothiazylsulfenamide (mercapto mix)	95-33-0	
Dibenzothiazyl disulfide (mercapto mix)	120-78-5	
2-mercaptobenzothiazole (mercapto mix)	149-30-4	
2-(4-morpholinyl mercapto)-benzothiazol (mercapto mix)	102-77-2	
Methylchloroisothiazolinone/methylisothiazolinone mix	55965-84-9	Data from methylisothiazolinone available
Tixocortol-21-pivalate	55560-96-8	
Mercaptobenzothiazole	149-30-4	
Colophony	8050-09-7	
Ethylenediamine dihydrochloride	333-18-6	
Lanolin alcohol (Amerchol 101)	8027-33-6	
Bacitracin	1405-87-4	
Dibucaine	85-97-0	
Parthenolide	20554-84-1	
Lidocaine	137-58-6	
Gold sodium thiosulfate	10233-88-2	
Disperse blue 106 (disperse blue m124/106 mix)	68516-81-4	
Disperse blue 124 (Disperse blue m124/106 mix)	61951-51-7	
Hydrocortisone-17-butyrate	13609-67-1	

ACDS Core Allergen Nickel(II) sulfate hexahydrate	CAS Number 10101-97-0	Comments
Hexyl cinnamic aldehyde (fragrance mix 2)	101-86-0	Data from other components of fragrance mix 2 available
Lyral (fragrance mix 2)	31906-04-4	Data from other components of fragrance mix 2 available
Cocamidopropyl betaine	61789-40-0	
Diethyl thiourea (mixed dialkyl thiosureas)	105-55-5	
Dibutyl thiourea (mixed dialkyl thiosureas)	109-46-6	
Oleamidopropyl dimethylamine	109-28-4	
Decyl glucoside	141464-42-8	
Amidoamine	Not available	
Melaleuca/tea tree oil	68647-73-4	
Chlorhexidine digluconate	18472-51-0	
Propolis	85665-41-4	
Tosylamide formaldehyde resin	1338-51-8	Data for tosylamide used
Alantolactone (sesquiterpine lactone mix)	546-43-0	
Costunolide (sesquiterpine lactone mix)	553-21-9	
Dehydrocostus lactone (sesquiterpine lactone mix)	477-43-0	
Cocamide DEA	68603-42-9	
Benzalkonium chloride	63449-41-2	
Ylang-Ylang	8006-81-3	
Anthemis nobilis extract (Compositae mix 2)	84649-86-5	
Chamomilla recutita extract (Compositae mix 2)	84082-60-0	
Achillea millefolium extract (Compositae mix 2)	84082-83-7	
Tanacetum vulgare extract (Compositae mix 2)	84961-64-8	
Arnica montana extract (Compositae mix 2)	68990-11-4	
Parthenolide (Compositae mix 2)	20554-84-1	
Dimethylol dihydroxy ethylene urea (ethyleneurea melamine formaldehyde mix)	1854-26-8	
Melamine formaldehyde (ethyleneurea melamine formaldehyde mix)	Not available	
Triamcinolone	76-25-5	
Clobetasol-17-proprionate	25122-46-7	
Disperse orange 3	730-40-5	
Jasminum officinale oil	8031-01-4	
White petrolatum	8009-03-8	